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Author(s): Gattiker, James R.

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Energy Systems Process Modeling, Analysis, and Experiment Design

James R. Gattiker
Los Alamos Statistical Sciences

Abstract

This presentation is to be used in Feynman Center outreach discussions. It describes public information about some Los Alamos interests and activities in modeling and analysis in energy systems including carbon capture and direct air capture. In particular this addresses the CCSI2 project's open-source toolkit and ongoing partnerships, as well as summarizing the published Feynman Center capability snapshot on direct air capture.

Model-Supported Science and Engineering in Energy Systems

Technology development is enhanced when co-developing with computational models and system experiments.

- Model-based insight into processes
- Model predictions of systems studied, and projected
- Experiment design and planning
- Uncertainty quantification

Through the CCSI2 project we have been working in accelerating engineered systems for post-combustion capture, by connecting basic properties models and data to at-scale models and experimental deployments.

We are connecting this capability to the separation and capture components of energy transition systems.

CCSI^2

Carbon Capture Simulation for Industry Impact

NATIONAL ENERGY TECHNOLOGY LABORATORY · Lawrence Livermore National Laboratory · Pacific Northwest National Laboratory · Berkeley Lab · Oak Ridge National Laboratory · West Virginia University · University of Notre Dame · The University of Texas at Austin

R&D 100 WINNER

- CCSI Toolset: Open-source models and analysis tools targeting capture process engineering, accelerating deployment
- Sorbent and solvent systems templates
  - "Gold-standard" MEA models and analysis shows the path from basic science to NC3 experimental campaign to scale-up TEA.
- Co-development with industry partners including GE, MTR, Fluor, RTI
- Current EY projects emphasize model-based Design of Experiments for industry partner field campaigns

RTI CRADA for solvent model development and analysis, supporting upcoming TCM experimental campaign

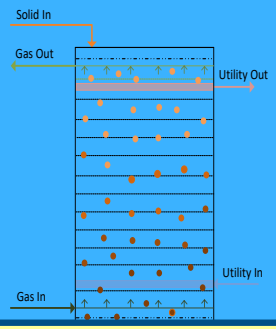
Technology Centre Mongstad

CCSI Toolset Workflow and Connections

acceleratecarboncapture.org

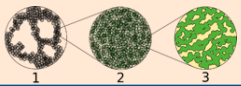
2016 Award

Process Models



Uncertainty

Basic Data Submodels



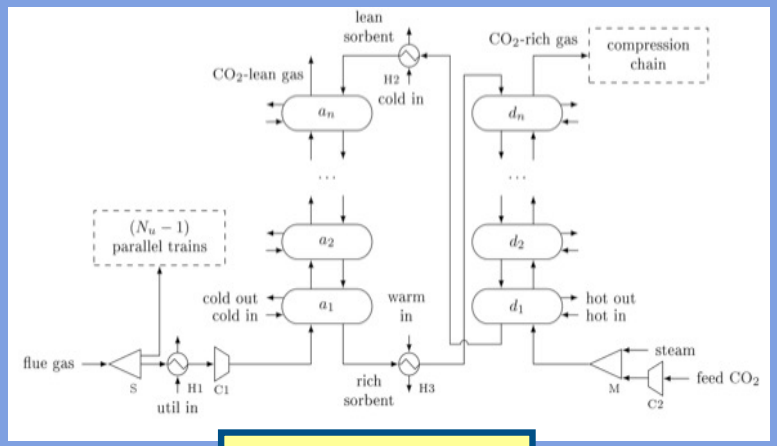
Uncertainty

Algebraic Surrogate Models

ALAMO

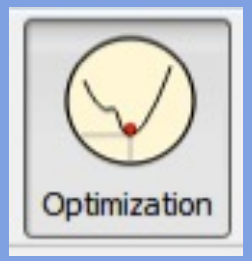
Uncertainty

Superstructure Optimization



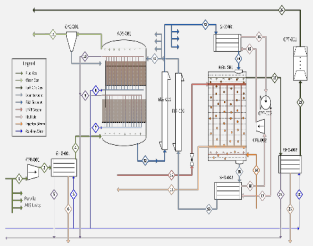
Uncertainty

Simulation-Based Optimization



Uncertainty

Optimized Process

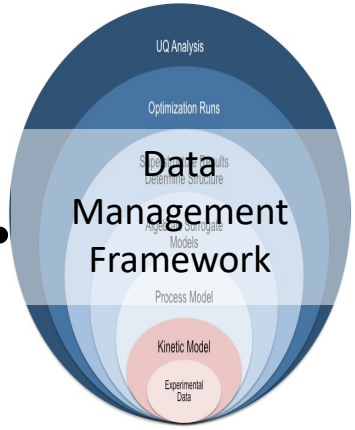


Uncertainty

Uncertainty Quantification

Process Dynamics and Control

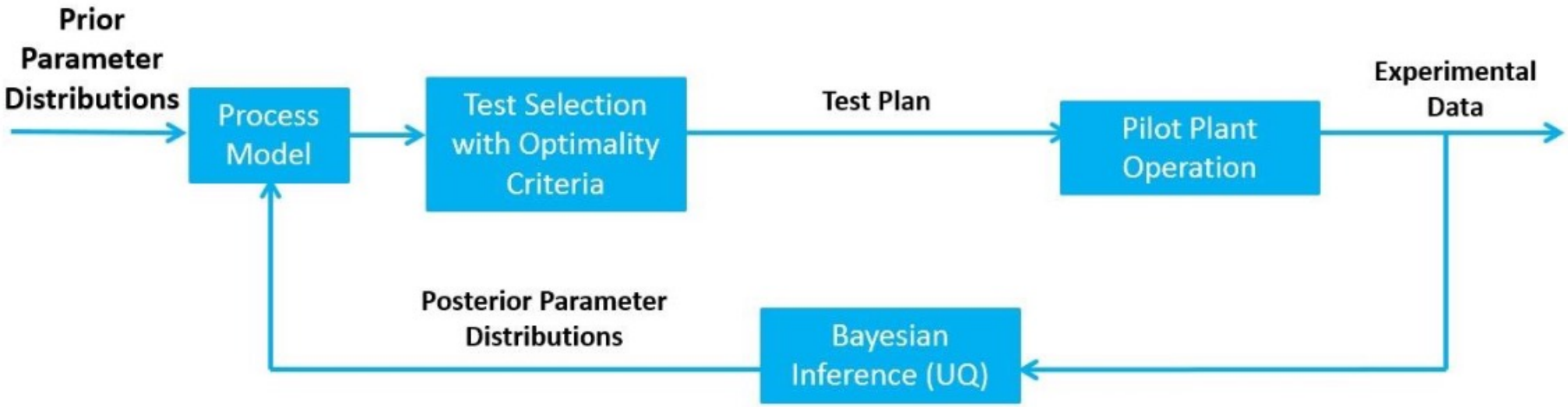
CFD Device Models



Technical Focus:
Sequential Design of Experiments

Payoff of models: Learn what we need to learn about for applied goals, e.g. reducing uncertainty in TEA

Provide tools and guidance to partners



Direct Air Capture: R&D, Testbeds, Partnering

Direct Air Capture is recognized as necessary for net-zero.

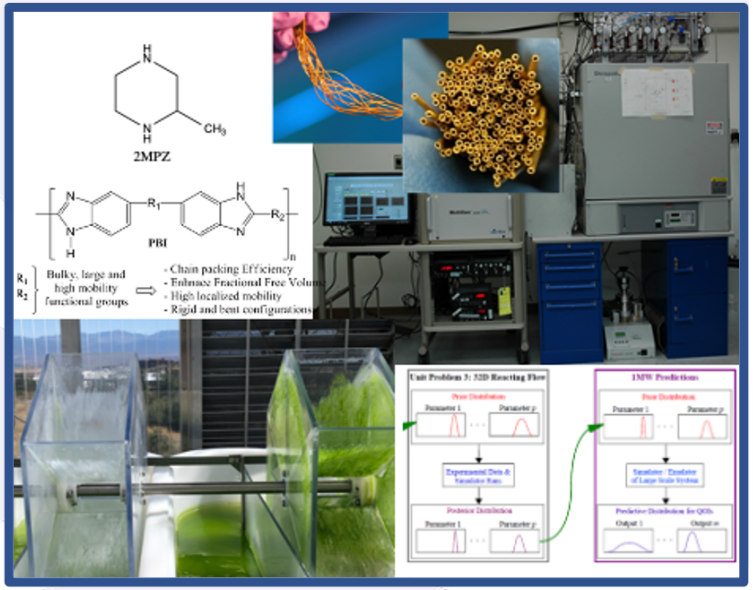
Los Alamos has a strong capability in separations, with membrane, solvent, and sorbent technologies.

Currently partnering:

- LANL testbeds and science-based models and analysis
- Partner project ownership, economics, and scale-up deployment

Experimentally validated models to evaluate, for example:

- Impact of CO2 levels and airflow, RH, T, technology-specific key parameters
- Reactant cycles
- Alternative chemical formulations
- Capture concept and handling alternatives



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